1,3-diphenyl-1,3-diazetidine
74949-76-1 | DTXSID60321268

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.42e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

Image not found
Heptachlor epoxide
Measured: 5.14e-07
Predicted: 3.52e-07

Image not found
Dieldrin
Measured: 5.80e-07
Predicted: 3.60e-07

Image not found
Endrin
Measured: 5.80e-07
Predicted: 3.60e-07

Image not found
Endrin aldehyde
Measured: 6.30e-08
Predicted: 1.07e-07

Image not found
N-(1-Naphthyl)ethylenediamine
Measured: 1.07e-02
Predicted: 9.11e-02

Image not found
Acridine
Measured: 2.14e-04
Predicted: 1.49e-05